



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 08:25 PM EDT

PDB ID : 5F3Y
Title : Crystal Structure of Myo7b N-MyTH4-FERM-SH3 in complex with Anks4b CEN
Authors : Li, J.; He, Y.; Lu, Q.; Zhang, M.
Deposited on : 2015-12-03
Resolution : 3.41 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

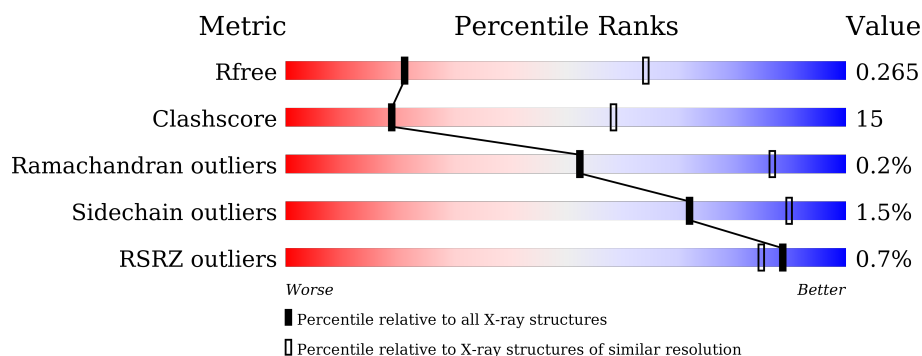
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	621	 63% 25% 12%
2	B	102	 7% 6% 87%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4041 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Unconventional myosin-VIIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	3951	2569	636	727	19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	958	GLY	-	expression tag	UNP Q99MZ6
A	959	SER	-	expression tag	UNP Q99MZ6
A	960	GLU	-	expression tag	UNP Q99MZ6
A	961	PHE	-	expression tag	UNP Q99MZ6

- Molecule 2 is a protein called Ankyrin repeat and SAM domain-containing protein 4B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	13	90	60	14	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	251	GLY	-	expression tag	UNP Q8K3X6

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	197.52Å 197.52Å 97.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.72 – 3.41 30.72 – 3.41	Depositor EDS
% Data completeness (in resolution range)	92.1 (30.72-3.41) 85.4 (30.72-3.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 3.39Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.241 , 0.280 0.225 , 0.265	Depositor DCC
R_{free} test set	1192 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 64.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 24790 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4041	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.42	0/4052	0.63	0/5577
2	B	0.28	0/91	0.48	0/123
All	All	0.41	0/4143	0.63	0/5700

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1062	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3951	0	3637	117	1
2	B	90	0	92	4	0
All	All	4041	0	3729	119	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:VAL:HG11	1:A:1162:PRO:HD3	1.70	0.74
1:A:1506:ASP:OD1	1:A:1529:ARG:NH1	2.21	0.74
1:A:1269:PHE:O	1:A:1412:TRP:HB3	1.88	0.73
1:A:1281:SER:O	1:A:1285:ILE:HG22	1.89	0.72
1:A:1389:ARG:HD3	1:A:1470:MET:HE2	1.71	0.72
1:A:1510:LEU:HD11	1:A:1541:LEU:HD13	1.72	0.71
1:A:1480:GLU:HG3	1:A:1516:LEU:HB2	1.73	0.71
1:A:1117:LEU:HD22	1:A:1149:LEU:HD13	1.71	0.69
1:A:1286:TYR:CE1	1:A:1375:THR:HG21	2.31	0.66
1:A:990:ILE:HG22	1:A:992:LYS:H	1.62	0.64
1:A:1395:THR:OG1	1:A:1403:LYS:O	2.14	0.61
1:A:1216:GLY:CA	1:A:1268:PHE:HB2	2.31	0.61
1:A:1181:ILE:HD12	1:A:1263:TYR:HE1	1.66	0.60
1:A:1224:TYR:HE1	1:A:1259:PRO:HG2	1.65	0.60
1:A:1009:ALA:O	1:A:1013:VAL:HG23	2.02	0.60
1:A:1272:TRP:CZ3	1:A:1477:GLY:HA3	2.36	0.60
1:A:1300:PHE:HZ	1:A:1309:LEU:HD12	1.67	0.60
1:A:1395:THR:HG22	1:A:1459:PHE:CE2	2.37	0.59
1:A:1500:LEU:HD13	1:A:1534:GLY:N	2.17	0.59
1:A:1228:TRP:HB3	2:B:274:VAL:HG12	1.85	0.59
1:A:1524:LEU:HB3	1:A:1535:LEU:HD23	1.84	0.59
1:A:1197:THR:HG22	1:A:1199:ARG:H	1.69	0.58
1:A:1122:PRO:HG3	1:A:1130:LEU:HD23	1.84	0.58
1:A:1480:GLU:O	1:A:1514:GLN:HG2	2.03	0.58
1:A:1448:LEU:HD22	1:A:1467:ILE:HD11	1.84	0.58
1:A:1290:LEU:HD13	1:A:1313:HIS:CE1	2.39	0.57
1:A:1224:TYR:CE1	1:A:1259:PRO:HG2	2.40	0.57
1:A:1269:PHE:CZ	1:A:1285:ILE:HD11	2.41	0.56
1:A:1178:ILE:HD13	1:A:1237:LEU:HD11	1.88	0.56
1:A:1159:ALA:N	1:A:1239:ASP:OD2	2.39	0.56
1:A:974:PRO:HA	1:A:987:HIS:CD2	2.40	0.56
1:A:1506:ASP:CG	1:A:1529:ARG:HH12	2.09	0.56
1:A:1393:VAL:HG22	1:A:1461:SER:HB3	1.88	0.56
1:A:1206:ALA:O	1:A:1210:GLY:N	2.39	0.55
1:A:1216:GLY:HA3	1:A:1268:PHE:HB2	1.90	0.54
1:A:983:LYS:O	1:A:984:SER:OG	2.25	0.54
1:A:1223:VAL:HG21	1:A:1244:CYS:SG	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1419:ASP:HB2	1:A:1423:ARG:O	2.07	0.53
1:A:1297:GLU:HA	2:B:268:PRO:HD2	1.90	0.53
1:A:1312:ARG:O	1:A:1316:VAL:HG23	2.09	0.53
1:A:1004:ASP:O	1:A:1005:THR:OG1	2.21	0.53
1:A:1126:PHE:CE2	1:A:1130:LEU:HB2	2.44	0.53
1:A:974:PRO:HA	1:A:987:HIS:HD2	1.75	0.52
1:A:1008:SER:O	1:A:1011:LEU:HG	2.09	0.52
1:A:1511:THR:OG1	1:A:1524:LEU:O	2.28	0.52
1:A:1122:PRO:HD3	1:A:1149:LEU:HD11	1.92	0.52
1:A:1271:PRO:HB2	1:A:1478:LEU:HD21	1.91	0.52
1:A:1517:LEU:HD12	1:A:1517:LEU:N	2.25	0.52
1:A:1394:THR:OG1	1:A:1460:VAL:O	2.27	0.51
1:A:1464:SER:HA	1:A:1467:ILE:HG12	1.92	0.51
1:A:1155:ASN:ND2	1:A:1200:GLU:OE2	2.39	0.51
1:A:1013:VAL:O	1:A:1017:ILE:HG13	2.11	0.51
1:A:1181:ILE:HD12	1:A:1263:TYR:CE1	2.45	0.51
1:A:1224:TYR:HE1	1:A:1259:PRO:CG	2.23	0.51
1:A:1500:LEU:HD12	1:A:1501:PRO:HD2	1.91	0.51
1:A:1004:ASP:O	1:A:1006:ASP:N	2.40	0.50
1:A:1526:GLN:HB3	1:A:1533:THR:HG22	1.93	0.50
1:A:1480:GLU:CD	1:A:1516:LEU:HD12	2.32	0.50
1:A:1340:TYR:OH	1:A:1345:PRO:HB3	2.11	0.50
1:A:1494:THR:HG22	1:A:1495:ASP:H	1.77	0.50
1:A:1089:ILE:O	1:A:1093:ILE:HG13	2.12	0.49
1:A:1285:ILE:O	1:A:1289:VAL:HG23	2.13	0.49
1:A:1394:THR:HG22	1:A:1405:GLN:HA	1.94	0.49
1:A:1399:PRO:O	1:A:1457:TYR:OH	2.26	0.49
1:A:1121:PRO:HD3	1:A:1157:VAL:HG22	1.93	0.49
1:A:1278:ASP:OD1	1:A:1280:VAL:N	2.45	0.49
1:A:1216:GLY:HA2	1:A:1268:PHE:HB2	1.95	0.48
1:A:1289:VAL:O	1:A:1293:VAL:HG23	2.14	0.48
1:A:1211:LEU:HD21	1:A:1217:PHE:CE2	2.48	0.48
2:B:263:SER:OG	2:B:264:ILE:N	2.48	0.47
1:A:1165:LEU:HD22	1:A:1176:ILE:HD13	1.96	0.47
1:A:1314:CYS:O	1:A:1318:LEU:N	2.46	0.47
1:A:1526:GLN:CB	1:A:1533:THR:HG22	2.44	0.47
1:A:1113:LEU:O	1:A:1117:LEU:HB2	2.15	0.47
1:A:1538:THR:HA	1:A:1541:LEU:HD12	1.96	0.47
1:A:1292:GLY:HA3	1:A:1298:TYR:CD2	2.50	0.46
1:A:1516:LEU:HD23	1:A:1516:LEU:O	2.15	0.46
1:A:1159:ALA:O	1:A:1160:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:MET:CG	1:A:1453:LEU:HD23	2.46	0.46
1:A:1516:LEU:HB3	1:A:1517:LEU:HD12	1.97	0.45
1:A:1372:ARG:O	1:A:1375:THR:HG22	2.16	0.45
1:A:1117:LEU:HD12	1:A:1145:CYS:HB3	1.97	0.45
1:A:1160:GLU:N	1:A:1239:ASP:OD2	2.49	0.45
1:A:1181:ILE:HB	1:A:1263:TYR:CD1	2.52	0.45
1:A:1271:PRO:HG2	1:A:1272:TRP:CE3	2.52	0.45
1:A:1393:VAL:HG22	1:A:1461:SER:CB	2.47	0.45
1:A:1494:THR:HG22	1:A:1495:ASP:N	2.32	0.45
1:A:999:LEU:HD12	1:A:1088:GLU:HA	1.98	0.45
1:A:1414:GLY:HA2	1:A:1430:PHE:CE2	2.52	0.45
1:A:1223:VAL:HG22	1:A:1260:TRP:CB	2.47	0.44
1:A:1369:LEU:O	1:A:1373:GLU:HG3	2.17	0.44
1:A:1192:VAL:HG13	1:A:1196:SER:HB2	1.98	0.44
1:A:1463:SER:O	1:A:1467:ILE:HG23	2.18	0.44
1:A:1550:PRO:CB	1:A:1554:LEU:HD12	2.47	0.44
1:A:972:THR:HG22	1:A:1132:ASN:OD1	2.18	0.43
1:A:998:LEU:N	1:A:1088:GLU:OE2	2.48	0.43
1:A:1272:TRP:CH2	1:A:1477:GLY:HA3	2.54	0.42
1:A:1510:LEU:HA	1:A:1510:LEU:HD23	1.51	0.42
1:A:1339:LEU:HA	1:A:1342:THR:HG23	2.01	0.42
2:B:265:LEU:HD22	2:B:273:ILE:HD11	2.01	0.42
1:A:1130:LEU:O	1:A:1134:ILE:HG13	2.19	0.42
1:A:1317:GLN:O	1:A:1318:LEU:HD23	2.19	0.42
1:A:1018:LEU:HB3	1:A:1024:LEU:HG	2.02	0.42
1:A:1393:VAL:HA	1:A:1461:SER:HB3	2.01	0.42
1:A:1272:TRP:CD1	1:A:1481:ARG:NH1	2.87	0.42
1:A:1406:LEU:HA	1:A:1406:LEU:HD23	1.76	0.42
1:A:1285:ILE:HG21	1:A:1285:ILE:HD13	1.71	0.42
1:A:1286:TYR:CE2	1:A:1372:ARG:HG2	2.55	0.42
1:A:1360:GLN:O	1:A:1363:GLN:N	2.34	0.42
1:A:1484:PHE:CE2	1:A:1549:LYS:HA	2.55	0.42
1:A:1026:GLU:HG2	1:A:1027:PRO:HD2	2.02	0.41
1:A:1517:LEU:H	1:A:1517:LEU:HD12	1.84	0.41
1:A:994:LEU:HD23	1:A:994:LEU:HA	1.92	0.41
1:A:981:PHE:HA	1:A:998:LEU:O	2.21	0.41
1:A:1286:TYR:CD2	1:A:1372:ARG:HG2	2.56	0.41
1:A:1117:LEU:HA	1:A:1117:LEU:HD23	1.93	0.41
1:A:1197:THR:HG22	1:A:1199:ARG:N	2.33	0.41
1:A:1408:LEU:HD23	1:A:1467:ILE:HD12	2.03	0.40
1:A:1223:VAL:HG12	1:A:1224:TYR:CD1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ARG:O	1:A:1344:SER:OG[8_555]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	541/621 (87%)	524 (97%)	16 (3%)	1 (0%)	52	87
2	B	11/102 (11%)	10 (91%)	1 (9%)	0	100	100
All	All	552/723 (76%)	534 (97%)	17 (3%)	1 (0%)	52	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1399	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	381/537 (71%)	375 (98%)	6 (2%)	70	89
2	B	10/88 (11%)	10 (100%)	0	100	100
All	All	391/625 (63%)	385 (98%)	6 (2%)	72	90

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	987	HIS
1	A	1234	CYS
1	A	1261	ARG
1	A	1348	TRP
1	A	1413	LYS
1	A	1481	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	549/621 (88%)	-0.43	3 (0%) 91 89	44, 88, 140, 188	0
2	B	13/102 (12%)	0.80	1 (7%) 16 16	130, 150, 173, 182	0
All	All	562/723 (77%)	-0.40	4 (0%) 89 85	44, 88, 145, 188	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1495	ASP	3.0
1	A	1322	VAL	2.5
2	B	266	ASN	2.2
1	A	1028	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.